

Carbon tetrachloride
56-23-5 | DTXSID8020250

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: -3.94 °C

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 3.01e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|--|
| <div>Image not found</div> <div>Carbon tetrachloride</div> <div>Measured: -23.0</div> <div>Predicted: -3.94</div> | <div>Image not found</div> <div>Hexachloroethane</div> <div>Measured: 187</div> <div>Predicted: 118</div> | <div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: -22.3</div> <div>Predicted: -13.3</div> |
| <div>Image not found</div> <div>Hexachloropropene</div> <div>Measured: -72.9</div> <div>Predicted: -34.7</div> | <div>Image not found</div> <div>Ethylamine-boron trifluoride</div> <div>Measured: 87.0</div> <div>Predicted: 73.8</div> | |